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Computational Investigation of Mass Sensing Using Defective Double Walled Carbon Nanotubes

Ajay M. Patel[a*], Anand Y. Joshi[b]

[a]*Associate Professor ,G. H. Patel College of Engineering & Technology, Vallabh Vidyanagar, Gujarat – 388120,India*
[b] *Professor ,G. H. Patel College of Engineering & Technology, Vallabh Vidyanagar, Gujarat – 388120,India*

Abstract

This manuscript explores the effect of defect like surface waviness in double walled carbon nanotube based Nano mass sensors. Experimental images have reported that double walled carbon nanotubes (DWCNTs) are not straight and that they have a significant amount of waviness associated with them. It is also detected that CNTs do not inherit the same wavy thickness throughout their length. Hence a constant curvature or radius model may give uniform thickness in terms of curvature throughout the length which may lead to erroneous results. In this paper resonant frequency shift of double walled carbon nanotubes with deviations along its axis and different boundary conditions namely cantilever and bridged have been investigated. It has been observed that the defect significantly contributes to the dynamics of carbon nanotubes.

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Keywords: DWCNT, Frequency Shift, Waviness, Mass Sensor

1. Introduction

Carbon nanotube (CNT), which was first discovered by Iijima et al(1991), have vast prospective for application as structural elements in nanoscale devices, owing to their remarkable mechanical, physical and chemical properties, such as low weight, high aspect ratio, extremely high stiffness, and highly sensitivity to their surroundings change [Dresselhaus, et al. (2004) and Wong, et al. (1997)]. Such features of CNTs make them auspicious candidates for atomic-resolution mass sensor, [Jensen and Kim (2008)].

Ajay M. Patel. Tel.: +91-942-703-7011; fax: +0-269-223-6896.
E-mail address:ajaympatel2003@yahoo.com

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Li and Chou (2003, 2004) studied the possible use of CNTs as nanoresonators and used the combined molecular structural mechanics and stiffness matrix methods to calculate the fundamental frequencies of CNTs for both cantilevered and bridged boundary conditions. Li and Chou (2004) also used this approach to determine the possible use of CNT-based nanomechanical resonators for mass detection. Natsuki et al (2008) applied wave propagation approach to vibration analysis of simply supported doubled-walled carbon nanotubes. DWCNTs are considered as a two-shell model coupled together the Van der Waals interaction between two adjacent nanotubes. Wang et al (2008) studied the group velocities of longitudinal and flexural wave propagations in single and multi-walled carbon nanotubes in the structure of continuum mechanics. Zhang et al (2001) applied the wave propagation approach to investigate the vibration frequencies of cylindrical shells filled with fluid.

Patel and Joshi (2013) analyzed vibrational characteristics of double walled carbon Nanotube (DWCNT) modelled using spring elements and lumped masses. The inner and outer walls of carbon Nanotube were modeled as two individual elastic beams interacting each other by van der Waals forces. To simulate the interlayer interactions and describe the van der waals potentials between carbon atoms on different layers appropriate spring elements are utilized. [Joshi et al (2010a)]. Moreover, Joshi et al (2010b) have reported that SWCNT based mass sensors exhibit super harmonic and sub harmonic response with different level of the mass.

In the review paper by Gibson et al. (2007), it has been indicated that different researchers have assumed, carbon nanotubes to be performing as perfectly straight beams or straight cylindrical shells. Likewise, as per the Scanning Electron Micrograph Joshi et al (2012) it is pretty clear that CNTs do possess some amount of waviness along its length. These tiny structures are not straight, but have certain degree of surface deviation or waviness with varying thickness along the length. The curved or wavy characteristic can be attributed to the manufacturing process used, in addition to mechanical properties such as low bending stiffness and large aspect ratio. The effect of waviness along the axis has been deliberate by subjecting the nanotube to different boundary conditions namely bridged, cantilever and simply supported and the vibration responses of straight and wavy DWCNTs are investigated by Patel and Joshi (2014).The results showed the sensitivity of the DWCNTs having different waviness to mass attached to tip of cantilever and centre of bridged DWCNTs and different length.

Nomenclature

R	Inter Atomic distance
ρ	Density of DWCNT
δ	Amplitude of waviness
x	special coordinate
Δr,	bond stretching increment
$\Delta\theta$	bond angle variation
$\Delta\phi$	angle variation of bond twisting

2. Modeling a DWCNT based nano sensor with waviness

It is difficult to model an actual experimental size DWCNT along with the surface waviness with varying thickness using a space frame model because of the huge number of elements and nodes required, but the Finite Element (FE) continuum model, if benchmarked properly, can solve that problem. The FE continuum model treats the DWCNT as a solid, continuous two thin-walled cylinders. Elemental level properties used in the FE models are the effective continuum properties, and depend upon the type of FE model used for benchmarking. While benchmarking against the results of Li and Chou's molecular structural mechanics approach, effective continuum properties E=1.1TPa, t= 0.3nm, and ρ=1.3g/cm3 are used. Effective continuum properties used for other standard cases have been extracted from Joshi et al (2010a).

For utilizing the finite element procedure potential energy is used to evaluate linear spring stiffness. The total force is the sum of the force generated by the electrons and the electrostatics force between positive charges. The general formula for the potential energy is

$$U = \sum U_r + \sum U_\theta + \sum U_\phi + \sum U_\omega + \sum U_{vdw} \quad (1)$$

Where, Ur is the energy due to bond stretch interaction, Uθ the energy due to bending (bond angle variation), UΦ the energy due to dihedral angle torsion, Uω the energy due to out-of plane torsion and Uvdw the energy due to non-bonded Vander Waals interaction.

$$U_r = \frac{1}{2}k_r(r - r_0)^2 = \frac{1}{2}k_r(\Delta r)^2 \quad (2)$$

$$U_\theta = \frac{1}{2}k_\theta(\theta - \theta_0)^2 = \frac{1}{2}k_\theta(\Delta\theta)^2 \quad (3)$$

$$U_\tau = U_\phi + U_\omega = \frac{1}{2}k_\tau(\Delta\phi)^2 \quad (4)$$

Where kr, kθ, and kT are the bond stretching, bond bending and torsional resistance force constants, respectively, while Δr, Δθ and Δø represent bond stretching increment, bond angle variation and angle variation of bond twisting, respectively.

The interlayer interaction is described by the van der Waals potential. The Lenard-Jones 6-12 potential is utilized to express the interaction of carbon atoms located on the different walls

$$U(R) = 4\varepsilon\left[\left(\frac{\rho}{R}\right)^{12} - \left(\frac{\rho}{R}\right)^{6}\right], \quad (5)$$

Where R is the inter atomic distance and $\varepsilon = 3.8655\times10^{-13}$ N nm and $\sigma = 0.34$ nm, respectively [Li and Chou (2004)].

In order to evaluate the vibration description of DWCNTs, equations are developed that describe the dynamic equilibrium of the Finite Element model. The element equation constructed by the global stiffness and mass matrices can be assembled.

The dynamics equation hence becomes

$$c(u_2 - u_1) = K_1 u_1 + M_1 \ddot{u}_1 \quad (6)$$

$$-c(u_2 - u_1) = K_2 u_2 + M_2 \ddot{u}_2 \quad (7)$$

Where K_1 and K_2 are stiffness matrices, M_1 and M_2 are mass matrices.

$$u_1 = Y_1 e^{i\omega t} \qquad u_2 = Y_2 e^{i\omega t} \quad (8)$$

Where u_1 and u_2 are the deflection of inner and outer tube, Y_1 and Y_2 are the vibrational amplitude and ω is the vibrational frequency.

The elemental equation for global system become

$$\begin{pmatrix} K_1 + c & -c \\ -c & K_2 + c \end{pmatrix}\begin{bmatrix} Y_1 \\ Y_2 \end{bmatrix} - \omega_n{}^2 \begin{pmatrix} M_1 & 0 \\ 0 & M_2 \end{pmatrix}\begin{bmatrix} Y_1 \\ Y_2 \end{bmatrix} = 0 \quad (9)$$

For the Finite Element Model of DWCNT, the Van der Waals force field between the interfacial layers is represented by a spring element COMBIN40, and attached mass is joined with outer nanotube using element SOLID186. The spring stiffness coefficient of Equations (2)-(4) are taken to be equal to $k_r = 6.52\times10^{-7}$ N nm^{-1}, $k_\theta = 8.76\times10^{-10}$ N nm rad^{-2} and $k_\tau = 2.78\times10^{-10}$ N nm rad^{-2} [Cornell et al, (1995)]. To model the interlayer interactions and describe the van der Waals potentials between carbon atoms on different layers COMBIN40 linear spring element is utilized.

3. Modeling of a wavy DWCNT

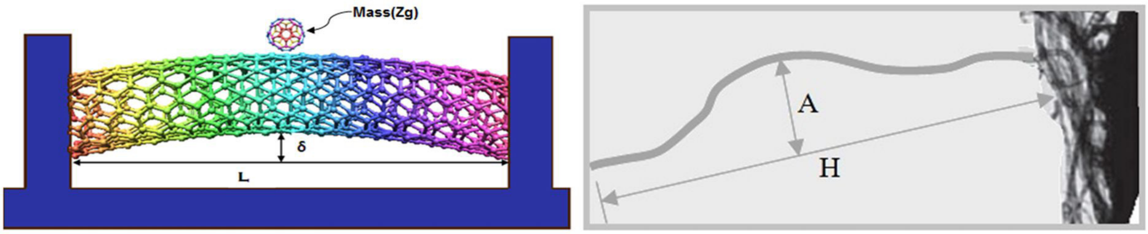
In the current study, the waviness associated with a DWCNT is defined by the waviness factor, Z=δ/L, where δ is the maximum amplitude of waviness and L is the projected length of the CNT. Figure 1(a) shows configuration of double wall carbon nanotube having waviness ratio defined as δ/L with attached mass. The surface deviation in DWCNT is described as a beam with an annular cross section having a large aspect ratio. The waviness in the nano beam is modeled using a half since wave with a small rise function described by

$$Z = \delta . \sin \frac{\pi x}{L} \tag{10}$$

Where x is the spatial coordinate, L is the length of the carbon nanotube and δ is the amplitude of its waviness. For the purpose of analysis the inner diameter and outer tube diameter are taken as 0.7nm and 1.4nm. The variation in waviness is taken within a range of 0.01 to 0.25. The length variations considered are L=10 nm, 15 nm, and 20 nm with mass attached 10^{-2} to 10^{4} Zg.

4. Results and discussion

The wavy cantilever and bridged DWCNT model that has been developed for the purpose of analysis is as under:
The inner diameter D1= 2R1 =0.7nm and outer tube diameter D2= 2R2 =1.4nm, where R1 and R2 are the inner and outer tube radius of the centre line. The DWCNT were assumed to have an elastic modulus of E= 1.1TPa (with Poisson ratio =0.25) and a density of = 1.3g/cm3. The effective thickness of DWCNT t=0.3nm.
Fig.1 (a) shows wavy bridged DWCNTs having attached mass outer wall and at the centre of the outer wall with the variation in the mass from 10^{-2} zg to 10^{4} zg. Figure 1(b) shows that waviness ratio associated with typical carbon nanotubes adopted by Zhang et al, (2001).



(a) (b)

Figure1 (a) DWCNT having waviness ratio δ/L with attached mass in (Zg) (b) Waviness ratio with typical nanotubes adopted by Zhang et al (2001).

Table 1 shows the frequency shift of wavy cantilever double walled carbon nanotube with waviness factor 0.1. It is clearly observed from the figure 2 (a) & (b) that with the increase in mass shorter length of CNTs exhibit a higher shift in the frequency. This suggests that irrespective of the type of boundary conditions shorter length CNTs are better candidates for mass sensing.

Table1. Frequency shift Wavy Cantilever DWCNT (D_2= 1.4nm, D_1=0.7nm and t=0.3) δ/L=0.1

Mass(Zg)	L= 10	L= 15	L= 20
0.01	0	0	0
0.1	8.38E+09	4.22E+09	3.16E+09
1	1.11E+10	5.58E+09	4.2E+09
10	1.19E+10	6.01E+09	4.53E+09
100	1.22E+10	6.14E+09	4.64E+09
1000	1.23E+10	6.19E+09	4.67E+09
10000	1.23E+10	6.2E+09	4.68E+09

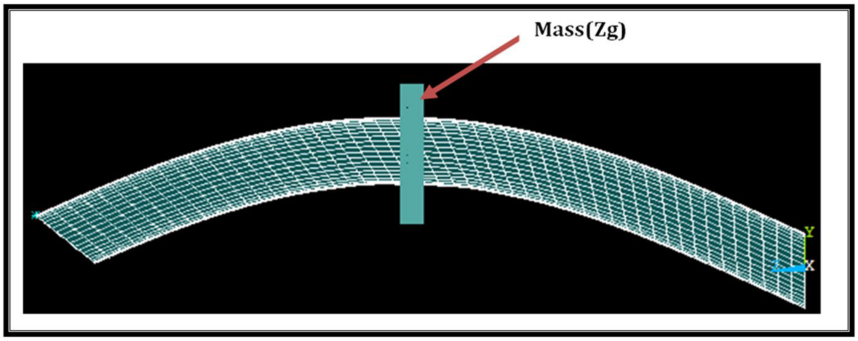


Figure 2. Finite Element Model of bridged DWCNT with waviness of δ/L=0.15, length 20nm and cylindrical mass added at the center.

Figure 2 shows the finite element model of Bridged DWCNT with a waviness of δ/L = 0.15 and length of 20 nm which has been modeled using the anisotropic material properties. The weak van der Waals force of attraction between the inner and the outer tubes has been modeled using the spring element COMBIN40.

Table2. Frequency shift Wavy bridged DWCNT (D_2= 1.4nm, D_1=0.7nm and t=0.3) δ/L=0.1

Mass(Zg)	L= 10	L= 15	L= 20
0.01	0	0	0
0.1	2.12E+10	1.35E+10	9.45E+09
1	2.81E+10	1.77E+10	1.22E+10
10	3.02E+10	1.91E+10	1.31E+10
100	3.09E+10	1.95E+10	1.34E+10
1000	3.11E+10	1.96E+10	1.35E+10
10000	3.12E+10	1.97E+10	1.35E+10

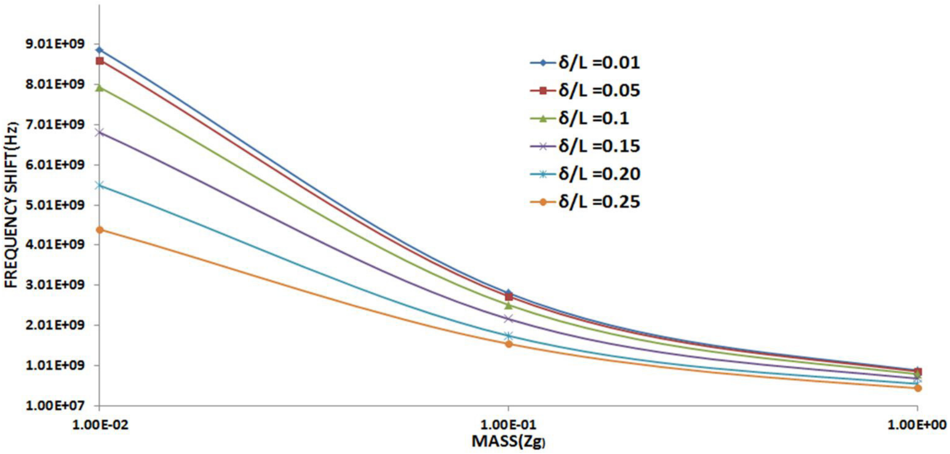


Figure3 Fundamental frequency shift vs. Mass (Zg) for various waviness (δ/L)

Figure 3 shows fundamental frequency shift vs. mass (Zg) for various waviness ratios. It is observed that a substantial shift in the Frequency takes place for lower values of waviness ratio which further reduces. This indicates that if change in the frequency is used for identifying the attached mass then lesser values of waviness ratios can predict the same with higher accuracy. Table 2 shows that frequency shift of wavy bridged DWCNT with waviness factor 0.1. Figure 4 (a) & (b) shows fundamental frequency of wavy cantilever and bridged DWCNT Resonator vs. Mass (Zg). It can be observed that the frequency shift is maximum for the bridged condition with a minimum length as compared to a cantilever end condition. This clearly suggests that the best end condition for mass sensors can be bridged and short CNTs are best suited for mass sensing.

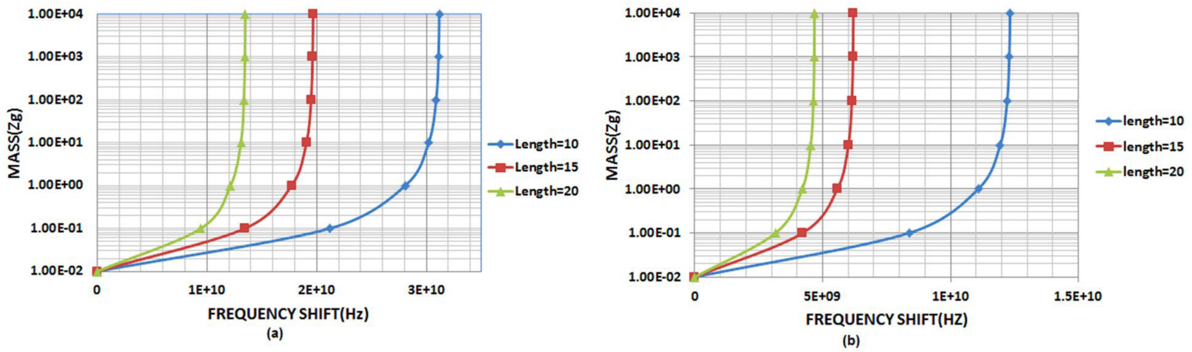


Figure 4 (a) &(b) Fundamental Frequency of wavy cantilever and bridged DWCNT Resonator vs. Mass (Zg)

5. Conclusion

- Effects of waviness indicate a reduction in the resonant frequencies with increase in the attached mass for both the configurations
- A higher value of frequency shift is detected with the increase in mass for smaller lengths of DWCNT as compared to larger lengths for a particular value of curvature factor as 0.1.
- Maximum frequency change is achieved for the bridged condition with a minimum length as compared to a cantilever end condition.

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